



## The microlocal Landau-Zener formula

Yves Colin de Verdière, Maurice Lombardi, Joël Pollet

### ► To cite this version:

Yves Colin de Verdière, Maurice Lombardi, Joël Pollet. The microlocal Landau-Zener formula. Annales de l'Institut Henri Poincaré Physique Théorique, 1999, 71 (1), pp.95. hal-00961343

**HAL Id: hal-00961343**

**<https://hal.science/hal-00961343>**

Submitted on 19 Mar 2014

**HAL** is a multi-disciplinary open access archive for the deposit and dissemination of scientific research documents, whether they are published or not. The documents may come from teaching and research institutions in France or abroad, or from public or private research centers.

L'archive ouverte pluridisciplinaire **HAL**, est destinée au dépôt et à la diffusion de documents scientifiques de niveau recherche, publiés ou non, émanant des établissements d'enseignement et de recherche français ou étrangers, des laboratoires publics ou privés.

**THE MICROLOCAL LANDAU-ZENER FORMULA  
(TO APPEAR IN ANNALES INSTITUT HENRI POINCARÉ  
(PHYSIQUE THÉORIQUE))**

YVES COLIN DE VERDIÈRE\*, \*\*  
MAURICE LOMBARDI\*\*\*  
JOËL POLLET\*\*\*

ABSTRACT. We describe the space of microlocal solutions of a  $2 \times 2$  system of pseudo-differential operators (PDO) on the real line near an avoided crossing (*2-levels system*). We prove Landau-Zener type formulae in the adiabatic case with avoided crossings and for the classical limit of coupled Schrödinger operators (Born-Oppenheimer approximation). The formulae that we get are uniform in the set of small parameters (Planck constant and coupling constant), they admits an uniquely determined complete asymptotic expansion and allow to access simply to phases which are needed in order to derive quantization conditions. The present paper is an expanded version of results already obtained by Joël Pollet in his PhD thesis [22]. Quantization conditions will be described in [5], following the techniques of [8]. See also [25] concerning the scattering matrix. An extension to time dependent Schrödinger equation close to the work by Hagedorn [13] and Hagedorn-Joye [14] and based on [20], [10] and [27] is also in preparation.

\* Institut Universitaire de France

\*\* Institut Fourier, UMR CNRS-UJF 5582

BP 74, 38402-Saint Martin d'Hères Cedex (France)

yves.colin-de-verdiere@ujf-grenoble.fr

\*\*\* Laboratoire de Spectrométrie physique, UMR CNRS-UJF 5588

BP 87, 38402-Saint Martin d'Hères Cedex (France)

maurice.lombardi@ujf-grenoble.fr

---

*Date:* March 10, 2011.

*1991 Mathematics Subject Classification.* 34C20, 34E20, 35Q40, 35S30, 81Q20.

*Keywords.* Pseudo-differential, semi-classic, microlocal, 2 levels system, Landau-Zener formula, adiabatic limit, Morse lemma.

## 1. INTRODUCTION

The origin of our work is a quantum mechanical problem: describe the behavior when  $h \rightarrow 0$  of the solutions of

$$(1) \quad \frac{h}{i} \frac{d\psi}{dt} = A(t)\psi,$$

where  $t \in \mathbb{R}$ ,  $\psi(t) \in \mathbb{C}^n$  or some Hilbert space, and  $A(t)$  is a linear operator (Hamiltonian) in that space. When  $A(t)$  has no crossing of eigenvalues, i.e. if the distance of one eigenvalue from the neighboring ones remains greater than some fixed (independent of  $h$ ) constant  $\delta$  for all  $t$ , then the main qualitative result is the *adiabatic approximation*: when  $h \rightarrow 0$ , if for some  $t_0$   $\psi(t)$  belongs to the eigenspace of such an isolated eigenvalue, it belongs to it for all  $t$ . Several levels of refinement can be found both in the physics and in the mathematics literature.

More precisely we will study the *breakdown* of the adiabatic approximation, i.e. what happens when two eigenvalues cross or nearly cross (the established name in the physical literature is *avoided crossings*) for some  $t_0$ . Qualitatively if  $\psi(t)$  belongs to the eigenspace of only one of those eigenvalues for  $t < t_0$ , it belongs to the direct sum of both for  $t > t_0$ , so one can define a *probability of transition* at the (avoided) crossing. The *Landau-Zener formula* for such a probability was established in 1932 in the physics literature [18, 29]. Better results were obtained the same year by Stückelberg [26]. In the mathematical literature the *Landau-Zener formula* in the *adiabatic regime* is proved for *analytic*  $A(t)$  in [12] and [15]. More refined formulae are given in [16]. The *Landau-Zener formula* for the semi-classical propagation of coherent states is proved by Hagedorn and Hagedorn-Joye ([13], [14]).

We will present here generalizations of a *Landau-Zener* type formula, valid for more general equations than those of quantum mechanics (i.e. optics, acoustics etc, for which there are little or no hints in the physics literature), and for less restrictive assumptions about operators than analyticity.

To grasp the principle of our method, it is first necessary to understand that this is a two *small* parameters problem, which must not be kept independent.

- the *adiabatic parameter*, which we will always denote  $h$ . It has nothing to do with the Plank's constant, but it is a renormalized non dimensional quantity, essentially the (small) ratio of the speed of variation as a function of  $t$  of the coefficients of  $A(t)$  and of the particular solution  $\psi(t)$  we want to study. Depending on the equation at hand, it can be  $\frac{S}{h}$ , ratio of the classical action and of the Plank's constant,  $(\frac{m}{M})^{1/4}$ , fourth square root of the ratio of the electron mass  $m$  and of a nuclear mass  $M$  (Born-Oppenheimer approximation), the reciprocal of the main quantum number or of the number of nodes of a wavefunction etc.

- the *coupling parameter*, which we will always denote  $\epsilon$ , essentially the minimum distance of the two eigenvalues at the (avoided) crossing position.

If one let  $h$  going to 0, with  $\epsilon$  fixed, one gets the *adiabatic* approximation, and corrections are *exponentially small* with respect to  $h$ . This is a particularly tricky

problem to handle, especially in the smooth, non analytic, framework. If one let  $\epsilon$  going to 0, with  $h$  fixed one gets the opposite *adiabatic* approximation and corrections as a perturbation theory with respect to  $\epsilon$ , less unwieldy because it is a regular perturbation theory. But we need a theory which interpolates smoothly between the two approximations, especially because it is frequently possible to go smoothly between the two limiting cases by varying an experimental parameter. This is what is given by the *Landau-Zener* formula: one gets a finite result when letting both  $h$  and  $\epsilon$  tend to zero, while keeping the ratio  $\frac{\epsilon^2}{h}$  constant.

Our theoretical framework will be the theory of pseudo-differential operators (PDO) with a small parameter  $h$  as presented in the book [23]. This is mainly because the limit  $h \rightarrow 0$  is the classical limit of quantum mechanics, and that this theory gives a mathematically sound way to tackle in quantum mechanics classical *phase space* properties: canonical transformations, *local in phase space* properties (called *microlocal* properties in this theory).

The basic idea will indeed be a classical phase space way of thinking, the same as that was used in [6, 7, 8]. The classical limit in phase space near an avoided crossing will be shown to be an Hamiltonian flow near a saddle point (fig. 1a). The classical way is to map with a canonical transformation  $\chi$  this flow to the Hamiltonian flow of  $y\eta - \Phi_0(\epsilon, h) = 0$ , where  $y$  and  $\eta$  are new conjugate coordinates and  $\Phi_0$  is some function we will compute (fig. 1b).

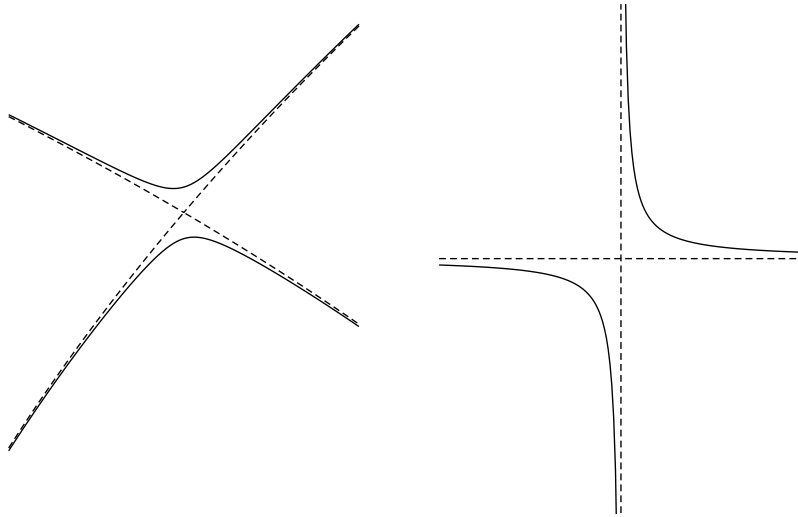


FIGURE 1. a) the original hamiltonian flow in phase space. b) the model hamiltonian flow after canonical mapping

The quantization of this new classical hamiltonian is:

$$(2) \quad H = \frac{h}{i} y \frac{d}{dy} - \Phi_0.$$

The crucial point is then that this **first order** differential equation has solutions which can be computed *exactly* in an elementary way [6].

All our work will be to give correct mathematical definitions and proofs to this loose way of thinking.

Let us be more precise. We will study a generalized 2-levels system in dimension 1 given by:

$$(3) \quad H_\epsilon \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} P_1(\epsilon, h) & \epsilon W(\epsilon, h) \\ \epsilon W^*(\epsilon, h) & P_2(\epsilon, h) \end{pmatrix} \begin{pmatrix} u \\ v \end{pmatrix} = 0.$$

Equation (1) is a particular case with  $H_\epsilon = \frac{h}{i} \frac{d}{dt} - A_\epsilon$ , where the dependance of the additional coupling parameter has been indicated. Here  $P_1, P_2$  and  $W$  are order 0  $h$ -PDO's which depends in a smooth way on  $\epsilon$  and the  $P_j$ 's are self-adjoint. We are located near a point  $z_0$  in the phase space  $T^*\mathbb{R}$  such that the principal symbols  $p_j$  of  $P_j$  vanish at  $z_0$  and their differentials at that point are linearly independent. We also assume that the principal symbol of  $W(0)$  at  $z_0$  does not vanish. Then  $\epsilon W(\epsilon)$  builds an *avoided crossing* of the eigenvalues of the principal symbol.

This general case covers 2 important particular cases:

**Example 1.1. : adiabatic Schrödinger equation.**

We consider the equation (1) where we assume

$$(4) \quad A_\epsilon(t) = \begin{pmatrix} \lambda_1(t) & \epsilon W(t) \\ \epsilon \bar{W}(t) & \lambda_2(t) \end{pmatrix},$$

and  $H_\epsilon = \frac{h}{i} \frac{d}{dt} \otimes \text{Id} - A_\epsilon(t)$ . We have then:

$$(5) \quad P_j = \frac{h}{i} \frac{d}{dt} - \lambda_j(t).$$

We assume that  $\lambda_1(t_0) = \lambda_2(t_0)$ ,  $\lambda_1'(t_0) \neq \lambda_2'(t_0)$  and that  $W(t_0) \neq 0$ . Then we have:

$$z_0 = (t_0, \lambda_1(t_0)).$$

It is also possible to solve the case of  $N$ -levels systems:

**Example 1.2. :  $N$ -levels systems.**

The motivation for looking at the very general situation of equation (3) is that the results apply also to any coupled system of  $N$  Schrödinger operators on the real line, near some avoided crossing of two of its eigenvalues. It is also possible to look at the adiabatic case (equation 1) for an  $N$ -levels system near an avoided crossing of two eigenvalues.

**Example 1.3. : semi-classical limit of a system a coupled Schrödinger operators.**

*It is a simple example of the Born-Oppenheimer approximation which is used as an approximation for quantum molecular dynamics.*

*The  $P_j$ 's are Schrödinger operators in one variable*

$$(6) \quad P_j = -\frac{h^2}{2} \frac{d^2}{dx^2} + V_j(x) - E$$

*and  $W$  is a nonzero complex number. We assume here that  $V_1(x_0) = V_2(x_0) < E$ ,  $V_1'(x_0) \neq V_2'(x_0)$  and we have  $z_0 = (x_0, \pm \sqrt{2(E - V_1(x_0))})$ .*

Let us start again with equation (3). We look at a point  $z_0$  which is a transversal intersection of the characteristic sets  $Z_j = \{p_j = 0\}$ ,  $j = 1, 2$ . The  $Z_j$ 's are oriented by the Hamiltonian vector fields of the  $p_j$ 's. We assume moreover that  $W(0)$  is *elliptic* at the point  $z_0$ . We denote by  $w_0$  the (non-zero) value of the principal symbol of  $W(0)$  at  $z_0$ .

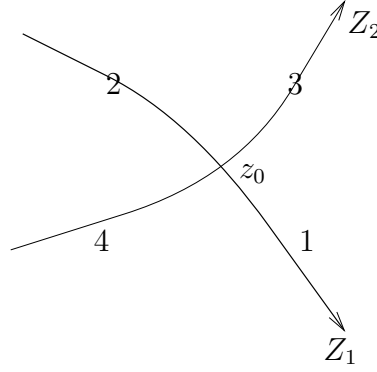


FIGURE 2. The  $Z_j$ 's and  $z_0$

We associate to that situation a transfer matrix

$$(7) \quad T = \begin{pmatrix} t_{1,2} & t_{1,4} \\ t_{3,2} & t_{3,4} \end{pmatrix}$$

which relates microlocal incoming solutions (that is roughly speaking WKB solutions on the 2 incoming edges) to outgoing solutions by the condition that they admit a prolongation as a microlocal solution near  $z_0$ . Such a matrix is unitary for *currents*  $J_\varphi^\pm$ . We compute explicitly the asymptotic expansions of the entries of  $T$  in an orthonormal basis of microlocal solutions on each edge. We get then a *Landau-Zener* type formula which we write

$$(8) \quad |t_{1,2}| = |t_{3,4}| + O(h^\infty) = \exp\left(-\frac{\pi}{h} \left( \frac{|w_0|^2}{|\{p_1, p_2\}(z_0)|} \epsilon^2 + O(\epsilon^3) + O(h\epsilon^2) \right)\right) + O(h^\infty).$$

In fact, we show more precisely that the argument in the exponential can be written  $\frac{\pi}{h}\Phi(\epsilon, h)$  where  $\Phi$  is a classical symbol with respect to  $h$  of the following type

$$\Phi \sim \sum_{k=0}^{\infty} \Phi_k(\epsilon) h^k$$

where the  $\Phi_k$ 's are smooth and satisfy  $\Phi_k(\epsilon) = O(\epsilon^2)$ .

For comparison with [19] (see in particular theorem 5.1) and with the existing literature, we mention the following facts:

- *The results are valid without any analyticity property.*
- *The results are local and even microlocal.*
- *We get a full asymptotic expansion with respect to both small parameters  $\epsilon$  and  $h$ .*
- *The results describe in an uniform way the transition between the coupled regime and the non coupled regime.*

The transition arises when  $\epsilon$  is of the same order as  $\sqrt{h}$ . If  $\epsilon \gg \sqrt{h}$  (domain II) the adiabatic approximation works ( $|t_{1,2}| = O(h^\infty)$ ) and we are then reduced to 2 scalar equations. If  $\epsilon \ll \sqrt{h}$  (domain I) the opposite, diabatic, approximation works: the 2 equations are uncoupled at the principal order.

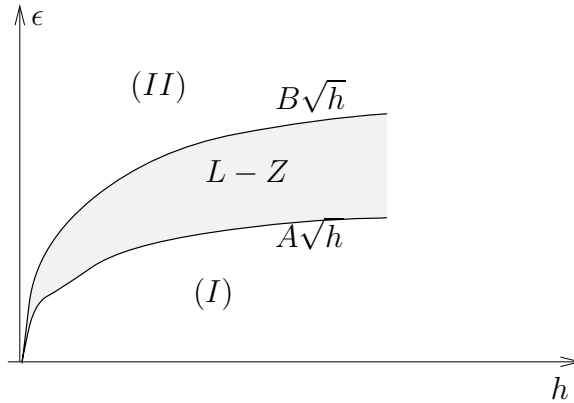


FIGURE 3. The parameters domain

Our way is to reformulate the *semi-classical Morse lemma* given in [6] in order that it holds for any deformation  $Q_\epsilon$  of a scalar PDO  $Q_0$  near a saddle point. The usual Morse lemma gives us some local coordinates which reduce a real valued function near a non degenerate critical point to its Taylor expansion at order 2. Some version with a given volume element (isochoric Morse lemma) has been derived in [9]. In the 2 dimensional case, it gives a symplectic version of the Morse lemma which asserts that there exists, near a saddle point, some Darboux's coordinates with respect to which the function can be written as  $f(y\eta)$ . It is then

rather easy to derive a semi-classical form of the Morse lemma by using Fourier integral operators in order to quantize this canonical transformation (see [6]).

Starting with the  $2 \times 2$  system given by equation (3), ellipticity of  $W$  at the point  $z_0$  allows to reduce to that kind of deformation for  $u$ , the following new equation (9) is called the *(non-commutative) determinant* of the system:

$$(9) \quad Q_\epsilon = WP_2W^{-1}P_1 - \epsilon^2WW^* .$$

We are then able to show that the equation  $Q_\epsilon u = 0$  is microlocally equivalent to

$$\left( \frac{h}{i} y \frac{d}{dy} - \Phi(\epsilon, h) \right) \tilde{u} = 0$$

near  $(0, 0)$ . This equation admits a 2 dimensional vector space of solutions which were carefully described in [6].

We get then an invariant associated to the system which is a formal series  $\Phi(\epsilon, h)$  with respect to both parameters  $h$  and  $\epsilon$ . To go back to the original space we need to consider a problem: the canonical transformation  $\chi_\epsilon$  which maps the two spaces is not unique. It maps level sets of  $q_\epsilon$  in the original space to level sets of  $y\eta - \Phi_0$  in the model space. But since the hamiltonian flow is a canonical mapping, composition of  $\chi_\epsilon$  by hamiltonian flow for any time  $t$  is an equally valid mapping. Even more, one can show that any smooth line of time origins  $t_0$  in the original space can be mapped to any smooth line in the model space. We thus need a proof that the final result in the original space is independent of this arbitrariness in the mapping. The proof comes from the fact that the resulting general Landau-Zener formula can be geometrically expressed as a cross-ratio: the space of microlocal solutions of the equation (3) has dimension 2 and the four subspaces of solutions microlocally vanishing on the four edges are four 1 dimensional subspaces of it. Their cross-ratio is our geometric invariant. In the unitary case, this cross-ratio determines the reflexion and transmission coefficients.

The scheme of the paper is the following: after some review of useful facts on cross-ratio's, we study a scalar equation which is a deformation of a case where the principal symbol has a saddle point (section 3); we give then a general statement for a coupled system of 2 PDO (section 4). In order to apply it to an  $N$ -levels adiabatic system, we need to use a reduction procedure which works into 2 steps: reduction from  $N$  to 2 levels (subsection 6.1) and reduction from 2 levels to 2 levels with  $t$ -independent non diagonal entry (subsection 6.2). We show how these results give Landau-Zener type formulae (section 6.3) for the adiabatic case and for the case of 2 coupled Schrödinger operators (section 5). At the end, we give some perspectives for the global case and for the case of arbitrary dimension.

## 2. CROSS-RATIO

Let  $K$  be a field, let  $E$  be a 2-dimensional vector space on  $K$  and  $P = P(E)$  the projective space of  $E$ , that means the set of 1 dimensional subspaces of  $E$ .



Let  $D_j$ ,  $j = 1, \dots, 4$ , be four elements of  $P$ , 3 of which are not equal. Let  $d$  be an affine line in  $E$  with  $0 \notin d$  and  $t \in K$  an affine parameter on  $d$ . We have the:

**Definition 1.** *The cross-ratio  $[D_1, D_2, D_3, D_4] \in K \cup \infty$  is defined in the following way. If  $t_j \in K \cup \infty$  are the parameters of  $D_j \cap d$ , we put:*

$$[D_1, D_2, D_3, D_4] = \frac{t_3 - t_1}{t_3 - t_2} : \frac{t_4 - t_1}{t_4 - t_2}.$$

The cross-ratio is independent of the choices of  $d$  and  $t$ .

In this paper,  $K$  will be the field of Laurent formal series with complex coefficients,  $E$  will be the space of microlocal solutions of our operator near the critical point  $z_0$ , and, if we number the 4 branches of the characteristic set  $Z_j$  for  $j = 1, 2, 3, 4$ , the  $D_j$ 's are the spaces of solutions which vanish microlocally on the  $Z_j$ 's. The fact that the  $D_j$ 's are 1 dimensional spaces and that no 3 of the  $D_j$ 's coincide depends on the result on normal forms (semi-classical Morse lemma, see theorem 1).

Let us assume that  $E \subset \oplus_{j=1}^4 E_j$ , where the  $E_j$ 's are 1 dimensional vector spaces on  $K$ , is the graph of a linear mapping  $T : E_1 \oplus E_2 \rightarrow E_3 \oplus E_4$ . We choose basis for the  $E_j$ 's and we assume that the matrix of  $T$  is  $(T) = (t_{i,j})$ . If  $D_j = E \cap H_j$  where  $H_j \subset E$  is the hyperplane whose projection on  $E_j$  is 0, then:

$$[T] = [D_1, D_2, D_3, D_4] = \frac{t_{2,3}t_{1,4}}{t_{1,3}t_{2,4}}.$$

**Proposition 1.** *If  $K = \mathbb{C}$  or  $\mathbb{C}(h)$ , if the  $E_j$ 's are Hilbert spaces and if  $T$  is unitary, we have  $[T] = 1 - \frac{1}{|t|^2}$ , where  $t$  is one of the diagonal elements of  $(T)$  where the matrix is computed in an orthonormal basis.*

### 3. DEFORMATIONS OF SADDLE POINTS

**3.1. The context.** Let  $p_j$ ,  $j = 1, 2$  be two smooth functions from  $T^*\mathbb{R}$  into  $\mathbb{R}$ . We assume that we are looking near a point  $z_0 \in T^*\mathbb{R}$  (*saddle point*) such that

$$(10) \quad p_1(z_0) = p_2(z_0) = 0 \text{ and the differentials } dp_1(z_0), dp_2(z_0) \text{ are independent.}$$

Let  $Q_\epsilon$ , where  $\epsilon$  is a real parameter which stays close to 0, an  $h$ -PDO of order 0 which depends in a smooth way on  $\epsilon$ . Let us denote by  $q_\epsilon$  the principal symbol of  $Q_\epsilon$  and assume that  $q_0 = p_1 p_2$ . We assume that  $q_\epsilon(z_0) \sim \omega_0 \epsilon^l$  with  $\omega_0 \neq 0$  and  $l \geq 1$ :  $\omega_0 \epsilon^l$  is then an equivalent at  $\epsilon = 0$  of the critical value of  $q_\epsilon$ .

**3.2. Normal forms.** The following theorem is a variant of the isochoric Morse lemma (see [9]) and its semi-classical version [6]. The benefit of this variant is that it does not use the functional calculus, neither the self-adjointness of the Hamiltonians (we will only use the fact that the principal symbol is real valued).

**Theorem 1. (a)** *There exists a smooth family of germs of canonical transformations  $\chi_\epsilon : (\mathbb{R}^2, O) \rightarrow (\mathbb{R}^2, z_\epsilon)$  and of functions  $e_\epsilon(y\eta)$  such that  $q_\epsilon \circ \chi_\epsilon = e_\epsilon(y\eta)(y\eta - \Phi_0(\epsilon))$ .*

*The smooth function  $\Phi_0$  is not unique, but its Taylor expansion*

$$\Phi_0(\epsilon) \sim \sum_{j=l}^{\infty} c_{0,j} \epsilon^j$$

*is. We have:*

$$c_{0,l} = \pm \frac{\omega_0}{|\{p_1, p_2\}(z_0)|} ,$$

*where the  $\pm$  sign is discussed in the section 3.3.*

**(b)** *There exists a FIO (Fourier integral operator)  $U_\epsilon$  associated to  $\chi_\epsilon$  and a PDO  $E_\epsilon$  elliptic at the point  $O$  such that we have microlocally near  $O$ :*

$$(11) \quad U_\epsilon^{-1} \circ Q_\epsilon \circ U_\epsilon = E_\epsilon \circ \left( \frac{h}{i} y \frac{d}{dy} - \Phi(\epsilon, h) \right)$$

*where  $\Phi$  is a symbol in  $h$  of the form*

$$(12) \quad \Phi \sim \sum_{k=0}^{\infty} \Phi_k(\epsilon) h^k$$

*The  $\Phi_k$ 's are smooth and admit uniquely determined Taylor expansions*

$$\Phi_k(\epsilon) \sim \sum_{j=0}^{\infty} c_{k,j} \epsilon^j .$$

**(c)** *If  $Q_\epsilon = P_2(\epsilon)P_1(\epsilon) + \Omega_\epsilon$ , with  $\Omega_\epsilon = O(\epsilon^l)$ ,  $\Phi_k(\epsilon) = O(\epsilon^l)$  and then*

$$\Phi = c_{0,l} \epsilon^l + O(\epsilon^{l+1}) + O(h\epsilon^l) .$$

**3.3. Sign of  $c_{0,l}$ .** Let us put  $e_0 = e_0(0)$ . We will use the following relations:

$$|\det(\text{Hess}(p_1 p_2))|^{\frac{1}{2}}(z_0) = |\{p_1, p_2\}(z_0)| = |e_0| ,$$

and

$$\omega_0 = -e_0 c_{0,l} .$$

We are left with the problem of finding the sign of  $e_0$  which is  $\pm$  according to the sign of  $H_0$  on the image by  $\chi_0$  of the quadrant  $\{y > 0, \eta > 0\}$ ; see the figure 4.

**3.4. Proof of theorem 1 : part (a).** The isochoric Morse lemma [9] gives the existence of canonical mappings  $\chi_\epsilon$  such that

$$q_\epsilon \circ \chi_\epsilon = f_\epsilon(y\eta)$$

where  $f_\epsilon$  is smooth and smoothly dependent of  $\epsilon$ ,  $f_0(0) = 0$ ,  $f'_\epsilon(0) \neq 0$ . Implicit function theorem asserts that  $f_\epsilon$  admit a zero  $\Phi_0(\epsilon)$  such that  $\Phi_0(0) = 0$ . We write then

$$f_\epsilon(t) = e_\epsilon(t)(t - \Phi_0(\epsilon)) .$$

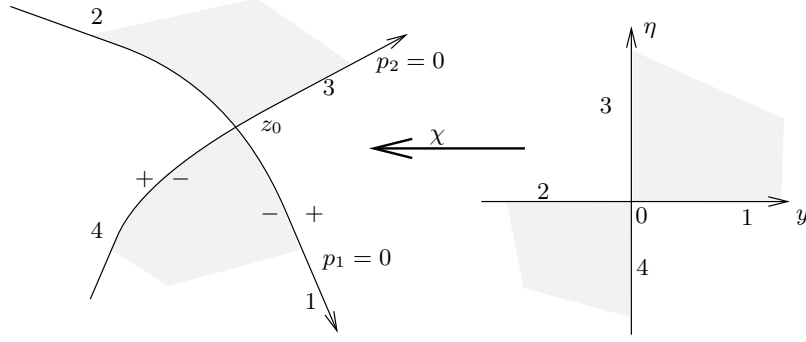


FIGURE 4. Numbering of branches and positivity domains of the Hamiltonians

The principle of the computation of  $\Phi_0(\epsilon)$  is to compare the areas limited by the original curve  $q_\epsilon=0$ , and the mapped curve  $y\eta = \Phi_0(\epsilon)$ , which must be equal since  $\chi_\epsilon$  is canonical. This would cause no problem for a node mapped to  $y^2 + \eta^2 = \Phi_0(\epsilon)$ , since these areas are finite, but needs a trick for our saddle case since they are both infinite.

We assume now that  $e_0(O) > 0$ . The way out is to use the existence of a singular asymptotic expansion (i.e. which contains some log terms) of

$$I_\varphi(\epsilon) = \int_{\{q_\epsilon \leq 0\}} \varphi |dx dy| = \int_{\{y\eta \leq \Phi_0(\epsilon)\}} \varphi \circ \chi |dy d\eta|$$

where  $\varphi$  is smooth and equal to 1 near  $z_0$ , we have:

$$I_\varphi(\epsilon) = -2\Phi_0(\epsilon) \log |\Phi_0(\epsilon)| + \Psi(\epsilon)$$

where  $\Psi$  is smooth. We have then

$$I_\varphi(\epsilon) \sim \sum_{k=1}^{\infty} (a_k \epsilon^k \log |\epsilon| + b_k(\varphi) \epsilon^k)$$

which gives the  $a_k$ 's (which are independent of  $\varphi$ ) from it we deduce the Taylor coefficients of  $\Phi_0$  by the identification

$$-2l\Phi_0(\epsilon) \sim \sum_k a_k \epsilon^k .$$

Notice that only the Taylor coefficients are determined that way, so that  $\Phi_0(\epsilon)$  is determined only up to a flat function of  $\epsilon$ , but it was shown in [9] that  $\chi$  is unique only up to a flat function.

**3.5. Proof of theorem 1 : part (b), existence.** Explicit dependencies on  $\epsilon$  will be omitted in this subsection. Let  $U$  be a FIO associated to  $\chi$ , Egorov's theorem gives:

$$(13) \quad U^{-1}QU = E(\Pi + R_1)$$

where  $E$  (resp.  $R_1$ ) is a PDO of order 0 (resp. 1), with principal symbol  $e$  (resp.  $r_1$ ). Also  $\Pi = \frac{h}{i}y\frac{d}{dy} - \Phi_0$ . We then look for  $P$ , a PDO of order 0 with principal symbol  $e^{is}$ , such that:

$$(14) \quad P^{-1}(\Pi + R_1)P = (\text{Id} + E_1)(\Pi - h\Phi_1 + R_2)$$

where  $E_1$  (resp.  $R_2$ ) are PDO of order 1 (resp. 2) and principal symbol  $e_1$  (resp.  $r_2$ ). Writing principal symbols of order 1 gives:

$$(15) \quad \{y\eta, s\} = -r_1 - \Phi_1 + e_1(y\eta - \Phi_0) .$$

where unknowns are  $s$ ,  $\Phi_1$  and  $e_1$ . It is known (see [12] or [6]) that such an equation can be solved iff there are no resonant terms, i.e. no powers of  $y\eta$  in its right hand side Taylor series. This gives an infinite set of equations for the  $e_1$  Taylor coefficients, and for  $\Phi_1$ ; if  $e_1 \sim \sum_{j=0}^{\infty} x_j(y\eta)^j$ , we must solve the system:

$$(16) \quad x_{j-1} - \Phi_0(\epsilon)x_j = r_j(\epsilon) \quad (j = 0, 1, \dots)$$

where  $x_{-1} = -\Phi_1$ . The  $r_j$ 's are the coefficients of  $(y\eta)^j$  in the  $r_1$  Taylor series. We solve this system using lemma 1 below. For that purpose set  $\Phi_0(\epsilon) = \beta$ , and look for  $x_j$  as  $C^\infty$  functions of  $\beta$ . The process is then iterated, conjugating with PDO's  $\text{Id} + S_l$ , where  $l = 1, \dots$ .

### 3.6. A lemma.

**Lemma 1.** *Let us consider the following (infinite) system of equations  $(\star_j)$ ,  $j \geq 0$  :*

$$(\star_j) \quad x_{j-1} - \beta x_j = a_j(\beta)$$

*where the  $a_j$ 's ( $j \geq 0$ ) are known as well as  $\beta$ , and the  $x_j$ 's ( $j \geq -1$ ) are unknowns. This system of equations has a solution  $x_j = f_j(\beta)$  where the  $f_j$ 's are smooth functions.*

*Proof.*—

Let  $f_{-1}$  be a smooth function whose Taylor series is  $f_{-1} \sim \sum a_j(\beta)\beta^j$ , where the  $a_j(\beta)$ 's are considered as formal series. We put  $x_{-1} = f_{-1}(\beta)$ ,  $x_0 = \frac{f_{-1}(\beta) - a_0}{\beta} \sim \sum a_{j+1}(\beta)\beta^j$ , and so on:  $x_k \sim \sum a_{j+k}(\beta)\beta^j$  is smooth.

□

**3.7. Proof of theorem 1 : part (c).** If  $Q_0 = P_1P_2$ , solutions of  $P_2u = 0$  give microlocal solutions of  $Q_0u = 0$  localized on the curve  $p_2 = 0$  and whose principal symbol does not vanish. It is compatible with the model

$$\frac{h}{i}y\frac{d}{dy} - \Phi(0, h) ,$$

(where  $p_2 = 0$  corresponds to  $\eta = 0$ ) only if  $\Phi(0, h)$  vanishes identically.

Let  $U_\epsilon$  be a FIO associated to  $\chi_\epsilon$  such that

$$U_\epsilon^{-1} P_2(\epsilon) P_1(\epsilon) U_\epsilon = E_\epsilon \circ \left( \frac{h}{i} y \frac{d}{dy} + O(h^\infty) \right).$$

We have then:

$$U_\epsilon^{-1} Q_\epsilon U_\epsilon = E_\epsilon \circ \left( \frac{h}{i} y \frac{d}{dy} + O(\epsilon^l) \right),$$

and we apply the proof given in section 3.5 (conjugation by PDO) which preserves the property of being  $O(\epsilon^l)$ .

**3.8. Cross-ratio and uniqueness.** The index  $\epsilon$  will often be implicit in what follows. Using [6], the dimension of the space  $\mathcal{E}$  of microlocal solutions of  $Pu = 0$  near  $z_0$  is 2 (as a module over the ring  $\mathbb{C}(h)$  of formal  $h$ -series). Let us label 1, 2, 3, 4 the 4 edges as in the figure (4) and let  $D_j \subset \mathcal{E}$  the line of solutions which vanish on the edge labelled  $j$ . We define  $m_{1,2,3,4} \in \mathbb{C}(h) \cup \infty$  as the cross-ratio of the four lines  $D_j$ .

**Theorem 2.** *We have:*

$$(17) \quad m_{1,2,3,4} = e^{-2\pi\Phi(\epsilon,h)/h} + O(h^\infty).$$

*There is a difficulty with the interpretation of this formula because  $\Phi = \Phi_0 + \Phi_1 h + \dots$ , so that we do not get a formal series. We split*

$$e^{-2\pi\Phi(\epsilon,h)/h}$$

*as a product of two terms*

$$e^{-2\pi\frac{\Phi_0(\epsilon)}{h}} e^{-2\pi(\sum_{j=1}^\infty \Phi_j(\epsilon) h^{j-1})} + O(h^\infty),$$

*the second one being now a formal series in the variable  $h$ . In particular, the  $(\epsilon, h)$ -formal series associated to  $\sum \Phi_k(\epsilon) h^k$  is uniquely determined.*

*Proof.*—

The formula comes from formula (38) in [6]. The transfer matrix  $T(\alpha)$  for the equation

$$\frac{h}{i} \left( y \frac{d}{dy} + \frac{1}{2} \right) - h\alpha$$

was given by

$$(18) \quad T(\alpha) = C(\alpha) \begin{pmatrix} 1 & -ie^{-\alpha\pi} \\ -ie^{-\alpha\pi} & 1 \end{pmatrix},$$

with there  $\alpha = \frac{E}{h}$  and here  $\alpha = \frac{\Phi}{h} + \frac{1}{2i}$ .

Uniqueness comes then from the geometric interpretation of  $m_{1,2,3,4}$  as a cross-ratio.

□

## 4. A COUPLED SYSTEM OF TWO HAMILTONIANS

Let us consider a semi-classical Hamiltonian

$$(19) \quad H_\epsilon = \begin{pmatrix} P_1(\epsilon) & \epsilon W(\epsilon) \\ \epsilon W^*(\epsilon) & P_2(\epsilon) \end{pmatrix}$$

where the  $P_j(\epsilon)$ 's (resp.  $W(\epsilon)$ ) are order 0  $h$ -PDO's on  $\mathbb{R}$  smoothly dependent on  $\epsilon$ , and whose principal symbols are  $p_j(\epsilon)$ 's (resp.  $w(\epsilon)$ ). The simplest case is that where  $P_1$  and  $P_2$  are two Schrödinger operators and  $W(\epsilon) = w$  with  $w$  a non-zero complex number. We define  $p_j = p_j(0)$ .

Let us assume that the  $p_j(\epsilon)$ 's are real valued and that there exists a point  $z_0$  such that  $p_j(z_0) = 0$  and the  $dp_j(z_0)$ 's are linearly independent. Let us assume that the principal symbols  $w(\epsilon, z_0)$  do not vanish at  $\epsilon = 0$ . We define  $w_0 = w(z_0, 0) \neq 0$ . We do not assume now that  $H_\epsilon$  is symmetric.

We are interested to microlocal solutions of

$$(20) \quad H_\epsilon U = 0 : \begin{cases} P_1(\epsilon)u + \epsilon W(\epsilon)v & = 0 \\ P_2(\epsilon)v + \epsilon W(\epsilon)^*u & = 0 \end{cases}$$

near  $z_0$ .

**4.1. Determinant operator.** Since  $W(\epsilon)$  is elliptic at the point  $z_0$ , it can be inverted, so that microlocal solutions of the system (20) near  $z_0$  are the solutions for  $\epsilon \neq 0$  of

$$(21) \quad \begin{cases} Q_\epsilon u & = 0 \\ v & = -\epsilon^{-1}W(\epsilon)^{-1}P_1u \end{cases}$$

with

$$(22) \quad Q_\epsilon = W(\epsilon)^*P_2W(\epsilon)^{-1}P_1 - \epsilon^2W(\epsilon)^*W(\epsilon) = \tilde{P}_2(\epsilon)P_1(\epsilon) - \epsilon^2W(\epsilon)^*W(\epsilon) .$$

The principal symbol  $q_\epsilon$  of  $Q_\epsilon$  is  $q_\epsilon = p_1(\epsilon)p_2(\epsilon) - \epsilon^2|w(\epsilon)|^2$  which has a saddle point  $z(\epsilon)$  with  $z(0) = z_0$ .

We can then use the results of the section 3 with  $l = 2$  and  $\omega_0 = -|w_0|^2$ .

**4.2. Currents and unitarity.** For a similar approach, see [19], §2. The difference is that we have not a global problem, and that unitarity must be microlocally defined.

The idea is to generalize the probability currents known in the physics literature on quantum mechanics [21]. Probability current at position  $x$  and time  $t$  for a quantum state described by the wave function  $\psi(x, t)$  is defined there as

$$(23) \quad \mathbf{J}(\psi) = \Re(\bar{\psi} \mathbf{p} \psi) = \Re(\bar{\psi} \frac{\hbar}{i} \frac{\mathbf{d}}{\mathbf{d}\mathbf{x}} \psi)$$

Using  $H = -\frac{\hbar^2}{2}\Delta + V(x)$  its divergence is computed as

$$(24) \quad \operatorname{div} \mathbf{J}(\psi) = \frac{i}{\hbar} [ \langle H\psi | \psi \rangle - \langle \psi | H\psi \rangle ],$$

so that time dependent Schrödinger equation leads to the fluid mechanics continuity equation:

$$(25) \quad \frac{\partial \rho}{\partial t} + \operatorname{div}(\mathbf{J}) = 0$$

where  $\rho = |\psi(x, t)|^2$  is the probability density, which justifies the interpretation of  $\mathbf{J}$  as a probability current.

Particularizing to the space-1d case, if  $\psi$  is a solution of  $H\psi = E\psi$ , thus  $|\psi|^2$  is time independent, integrating between two abscissae gives:

$$(26) \quad 0 = \frac{i}{h} \int_a^b (\langle H\psi | \psi \rangle - \langle \psi | H\psi \rangle) dx = [J(\psi)]_a^b$$

the first equation being due to self-adjointness of  $H$  ( $E$  is real), the second to integration by parts. Self-adjointness of  $H$ , which implies unitarity of the time evolution operator, and thus the time conservation of total probability, implies also that probability current that flows at  $a$  in a steady state situation is conserved at  $b$ .

The definition (23) is however heavily dependant on the particular form of the Schrödinger equation, whereas these considerations must be more general. Even in quantum mechanics, the consistency of the statistical interpretation implies the existence of a probability current in momentum space, which is not given by the analogous of the transparent eq. (23), except in the harmonic oscillator case. In fact the Stokes formula implicit in eq. (26) means that the proper definition of current is the  $(d-1)$ -differential form whose exterior derivative is the  $d$ -dimensional form integrated in the middle term. This form exists locally because a maximum dimensional form is closed.

Our definition (28) will short-circuit this evaluation, however, and will be valid for any  $H$ . The principle is contained in the transport equation solved for computing the amplitude  $A(x)$  to first order in  $\hbar$ , which is basically an equation of conservation of probability. For a *scalar* Hamiltonian the half density  $a(x)\sqrt{dx}$ , pulled up to the Lagrangian  $H(x, \xi) = 0$ , which in the 1d case is a curve parametrized by  $t$ , by

$$(27) \quad a(x)\sqrt{dx} = a(t)\sqrt{dt}$$

is solution of

$$\frac{1}{i} \frac{d}{dt} a(t) + \operatorname{sub} H(t) a(t) = 0$$

so that

$$a(t) = a(0) \exp \left( -i \int_0^t \operatorname{sub} H(s) ds \right)$$

so that for *real*  $\operatorname{sub} H$ , this introduces only a phase shift, but  $|a(t)|^2$  is conserved. This is thus the right definition of the current, which can be projected in  $x$ ,  $p$  or any other phase space coordinate by equation (27). Notice that the scalar

determinant operator  $Q_\epsilon$  defined in (22) has an *imaginary* sub-principal symbol, and thus do not conserve  $|a(t)|^2$ , because this operator acts on  $u$  only, and that some probability is transferred to  $v$ . The conservation of current is contained in the original matrix equation for *self-adjoint*  $H$ .

Let  $H$  be a (formally) self-adjoint matrix of PDO's on  $\mathbb{R}$ , with principal symbol  $H_0(x, \xi)$ , a Hermitian  $n \times n$  matrix, and with vanishing sub-principal symbol. We study the neighborhood of a point  $z_0 = (x_0, \xi_0) \in T^*\mathbb{R}$ , such that  $\ker(H_0(z_0))$  has dimension  $k$ , and suppose that near  $z_0$ ,  $H_0(z)$  admits  $k$  eigenvalues  $p_1, \dots, p_k$   $C^\infty$  which vanish at  $z_0$ . Let us assume that  $p'_j(z_0) \neq 0$  (but do not assume that the differentials are linearly independent) and (for simplicity) that  $z_0$  does not belong to the caustics of any of these  $p_j$ . Let  $[a, b]$  be a neighborhood of  $z_0$  which does not meet any of the caustics of the  $\mathcal{B}_j$ , where the  $\mathcal{B}_j$  are the curves  $p_j = 0$ . Let  $\mathcal{X}_j$  be the Hamiltonian flows of  $p_j$ , and  $dt_j$  be the differential on  $\mathcal{B}_j$  associated to the flow  $\mathcal{X}_j$  ( $dt(\mathcal{X}_j) = 1$ ). The image of  $dt_j$  by the projection onto the line

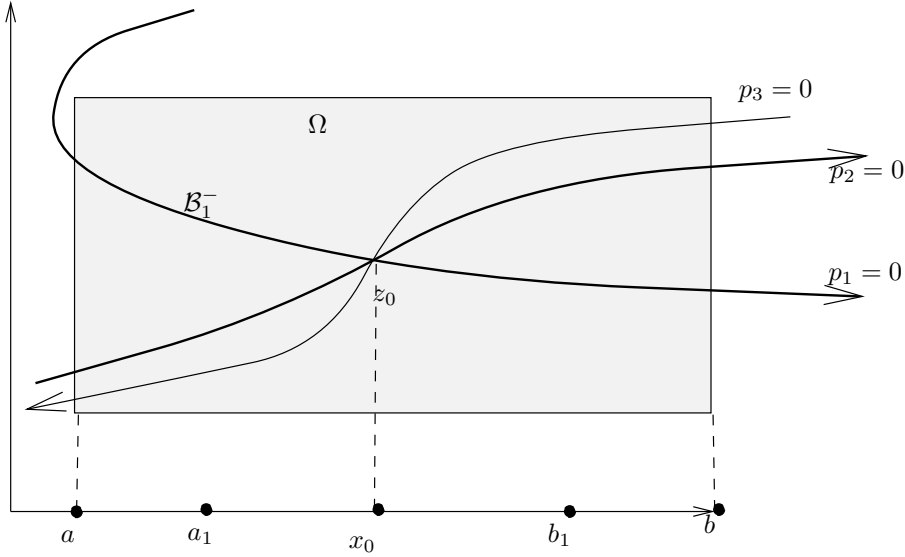


FIGURE 5. Currents ( $k = 3$ )

$\xi = 0$  is given by  $\pi_*(dt_j) = \frac{\partial p_j}{\partial \xi} dx$ . Let  $a < a_1 < x_0 < b_1 < b$  and  $\varphi \in C^\infty_0(]a, b[)$ , equal to 1 on  $[a_1, b_1]$ . Let moreover  $\Omega = [a, b] \times [c, d]$  be a rectangle containing the branches  $\mathcal{B}_j$ , which meets the characteristic manifold of  $H_0$  only on these branches.

**Definition 2.** Let  $U, V$  be two microlocal solutions within  $[a, a_1] \times [c, d]$  of  $HU = HV = O(h^\infty)$ . Define the left hand side **currents**

$$(28) \quad J_\varphi^-(U, V) = \frac{i}{h} \int_a^{a_1} \langle H(\varphi U) | \varphi V \rangle - \langle \varphi U | H(\varphi V) \rangle dx$$



and similarly, if  $U, V$  are two microlocal solutions within  $[b_1, b] \times [c, d]$ , the right hand side currents  $J_\varphi^+(U, V) = \frac{i}{h} \int_{b_1}^b \dots$ . Here  $\langle . | . \rangle$  is the pointwise Hermitian scalar product.

We have then the

**Theorem 3.** a) If  $U$  and  $V$  are microlocal solution in the whole  $\Omega$ :

$$J_\varphi^+(U, V) + J_\varphi^-(U, V) = O(h^\infty).$$

b) If  $U$  and  $V$  have microsupports in  $[a, a_1] \times [c, d]$  contained in two distinct  $\mathcal{B}_j$  branches:

$$J_\varphi^-(U, V) = O(h^\infty).$$

c) If the WKB form of  $U$ , assumed microlocalized on the branch  $\mathcal{B}_j$ , in  $[a, a_1]$  reads:

$$U(x) = A_j(x)e^{\frac{i}{h}S_j(x)} + O(h),$$

then:

$$(29) \quad J_\varphi^-(U, U) = (||A_j||^2 \frac{dx}{dt_j})(x') + O(h),$$

where  $x'$  is any point  $\in [a, a_1]$ .

The same holds for  $J_\varphi^+$ , with a change of sign. Suppose moreover that the dimension of the space of microlocal solutions in  $\Omega$  is  $k$  (this is true for  $k = 2$ , when supposing that the branches are transverses at  $z_0$ ). Let  $\mathcal{H}_-$  (resp.  $\mathcal{H}_+$ ) be the direct sum of the WKB solutions on the branches  $\mathcal{B}_j$  before  $z_0$  (for the Hamiltonian flows of the  $p_j$ 's) (resp. after). Then  $J_\varphi^\pm$  induces an Hilbert structure on  $\mathcal{H}_-$ , and the same holds for  $-J_\varphi^\pm$  on  $\mathcal{H}_+$ . Then every element  $\Phi_-$  of  $\mathcal{H}_-$  extends as an unique microlocal solution in  $\Omega$ , and the corresponding element in  $\mathcal{H}_+$  is denoted  $\Phi_+$ . The mapping  $\Phi_- \rightarrow \Phi_+$  is unitary modulo  $O(h^\infty)$  for the previous Hilbert structures.

*Proof.*—

a) On  $[a_1, b_1]$ :

$$H(\varphi U) = H(U) + O(h^\infty) = O(h^\infty)$$

and  $V$  has polynomial growth with respect to  $h^{-1}$ . Then:

$$J_\varphi^+(U, V) + J_\varphi^-(U, V) = \int_a^b \langle H(\varphi U) | V \rangle - \langle U | H(\varphi V) \rangle dx = O(h^\infty).$$

b) This is an elementary consequence of the stationary phase formula:

$$\int e^{i(S'_j(x) - S'_k(x))/h} a(x) dx$$

is  $O(h^\infty)$  if  $a \in C_o^\infty$  and  $S'_j - S'_k$  does not vanish on  $\text{Supp}(a)$ .

c) Let  $U(x) = A_j(x)e^{iS_j(x)/h} + O(h)$  be a WKB solution in  $[a, a_1]$ . The result follows easily from the computation of  $H(\varphi U)$  up to first order in  $h$ . The simplest way to do it is by using a reduction lemma as follows :

**Lemma 2.** *Let  $D$  be a domain in the phase space such that the principal symbol admits for any  $(x, \xi) \in D$  a non degenerate eigenvalue  $\lambda_0(x, \xi)$  smoothly dependent of  $(x, \xi)$ . Then there exists an unitary PDO  $P$  in  $D$  which satisfies*

$$(30) \quad P^{-1}HP = \begin{pmatrix} L & 0 \\ 0 & K \end{pmatrix}$$

where  $L$  is a self-adjoint operator whose principal symbol is  $\lambda_0(x, \xi)$ .

The proof of this lemma follows the same lines as the proof of theorem 5.

Then  $U = PV$  where  $V = a(x)e^{\frac{i}{h}S_j(x)}\epsilon_1 + O(h)$  where  $\epsilon_1 = (1, 0, \dots, 0)$  and  $\psi(x) = a(x)e^{\frac{i}{h}S_j(x)}$  satisfies  $L\psi = O(h^2)$ . We use then the usual transport equation which shows that  $|a(x)|^2 \frac{dx}{dt}$  is constant :  $L$  is self-adjoint and then his subprincipal symbol is real. Now  $A_j(x) = P_0(a(x)\epsilon_1)$  where  $P_0$ , the principal symbol of  $P$ , is a unitary matrix. The current is then computed by:

$$J_\varphi^-(U) = \int_a^{a_1} 2\varphi \frac{d\varphi}{dx} (||A_j||^2 \frac{dx}{dt_j})(x) dx .$$

□

**4.3. The generalized Landau-Zener formula.** Let  $E_j$ ,  $j = 1, \dots, 4$  be the spaces of microlocal solutions of  $H_\epsilon U = 0$  (equation 19) on the edges  $j$  (see figure 4).  $E_- = E_2 \oplus E_4$  and  $E_+ = E_1 \oplus E_3$  are Hermitian spaces for products defined using currents and if  $\mathcal{E}$  is the space of microlocal solutions near  $z_0$ ,  $\mathcal{E}$  is the graph of an unitary  $T$  map from  $E_-$  into  $E_+$ .

**Theorem 4.** *(generalized Landau-Zener formula) In an orthonormal basis for currents, we have*

$$T = (t_{i,j})$$

with :

$$|t_{1,2}| = |t_{3,4}| + O(h^\infty) = e^{\pi\Phi(\epsilon^2, h)/h} + O(h^\infty) .$$

where  $\Phi \sim \sum_{k=0}^\infty \Phi_k(\epsilon)h^k$  ( $\Phi_k \in C^\infty$  and  $\Phi_k(\epsilon) = O(\epsilon^2)$ ) satisfies:

$$\Phi(\epsilon, h) = -\frac{|w_0|^2}{|\{p_1, p_2\}(z_0)|} \epsilon^2 + O(\epsilon^3) + O(h\epsilon^2) .$$

The proof is a simple application of proposition 1.

If the  $P_j$ 's and  $W$  are  $\epsilon$ -independent,  $\Phi(\epsilon, h)$  is an even function of  $\epsilon$ . It allows to get a better remainder estimate:  $O(\epsilon^3)$  can be replaced by  $O(\epsilon^4)$ .

## 5. COUPLED SYSTEM OF TWO SCHRÖDINGER OPERATORS

We will now consider the system (3) where

$$P_j = -\frac{h^2}{2} \frac{d^2}{dx^2} + V_j(x) - E$$

are two Schrödinger operators and  $W = W(x)$  with  $W(x_0) = w_0 \neq 0$ . We assume that there exists  $x_0$  such that  $V_1(x_0) = V_2(x_0)$  et  $V'_1 = V'_1(x_0) \neq V'_2 = V'_2(x_0)$  and that  $E > V_j(x_0)$ . We have then

$$z_0 = (x_0, \pm \sqrt{2(E - V_j(x_0))}) = \pm \xi_0 \text{ .}$$

We apply theorem 4 and we get:

$$c_{0,1} = -\frac{|w_0|^2}{|\xi_0| |V'_1 - V'_2|(x_0)}$$

and because  $\Phi$  is even with respect to  $\epsilon$ ,  $\Phi = c_{0,1}\epsilon^2 + O(\epsilon^4) + O(h\epsilon^2)$ . This is the original (restricted) Landau-Zener formula.

## 6. ADIABATIC LIMIT WITH AVOIDED EIGENVALUES CROSSINGS

The adiabatic theorem in quantum mechanics is valid with the hypothesis that there are no eigenvalues crossings (see [2]). If two eigenvalues cross transversally, the adiabatic theorem remains true concerning the main term (see [1]) and there is a correction which is known as the Friedrichs-Hagedorn formula (see [11]). The Landau-Zener formula applies to avoided crossing of the order of  $\sqrt{h}$ . It was already remarked in [19] that there is an interpolating formula between both under some analyticity hypothesis. Our method provides a new way to attack this problem in the smooth case. We will start with an arbitrary  $N$ -levels system which fulfills some geometric hypothesis which is satisfied in the generic case.

Let us start with the equation:

$$(31) \quad \frac{h}{i} \frac{dX}{dt} = A_\epsilon(t)X, \quad a \leq t \leq b$$

where, for all  $t \in [a, b]$ ,  $A_0(t)$  is an  $N \times N$  Hermitian matrix,  $h > 0$  is the small *adiabatic parameter* and  $\epsilon$  is the small *coupling parameter*.

We assume that the following property holds: there exists  $t_0 \in ]a, b[$  such that  $A_0(t_0)$  admits an eigenvalue  $\lambda_0$  of multiplicity 2. We will denote by  $E_0$  the corresponding eigenspace. We will denote by  $n$  the Morse index of  $A_0(t_0) - \lambda_0 \text{Id}$  and by  $D_n$  the codimension 3 manifold of Hermitian matrices which admits the following type of spectrum:

$$\nu_1 \leq \dots \leq \nu_{n-1} < \nu_n = \nu_{n+1} < \dots \text{ .}$$

We will assume the following transversality hypothesis:

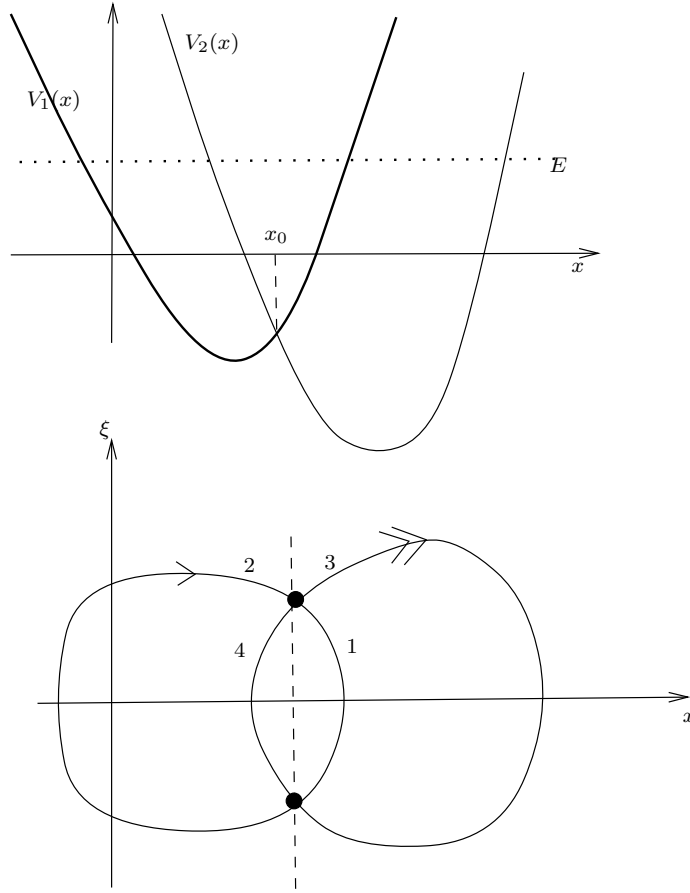


FIGURE 6. System of 2 Schrödinger operators

(**H**<sub>1</sub>): the smooth parametrized surface  $(t, \epsilon) \rightarrow A_\epsilon(t)$  is embedded into the space of  $N \times N$  Hermitian matrices and it is not tangent at the point  $A_0(t_0)$  to the codimension 3 manifold  $D_n$  (see figure 7).

The hypothesis (**H**<sub>1</sub>) can be reformulated in terms of the partial derivatives of  $A_\epsilon(t)$  at  $t = t_0$ . Let us define

$$\Omega_0 = \left\langle \frac{d}{dt} A_0(t) \Big|_{t=t_0} \cdot \Big| \cdot \right\rangle_{|E_0}$$

and

$$G_0 = \left\langle \frac{d}{d\epsilon} A_\epsilon(t_0) \Big|_{\epsilon=0} \cdot \Big| \cdot \right\rangle_{|E_0} .$$

The hypothesis (**H**<sub>1</sub>) is equivalent to the fact that  $\Omega_0$ ,  $G_0$  and Id are linearly independent.

We will assume that  $[a, b]$  is so small that the two eigenvalues  $\lambda_1(t)$  and  $\lambda_2(t)$  which prolong  $\lambda_0$  are distinct and separated from the rest of the spectrum.

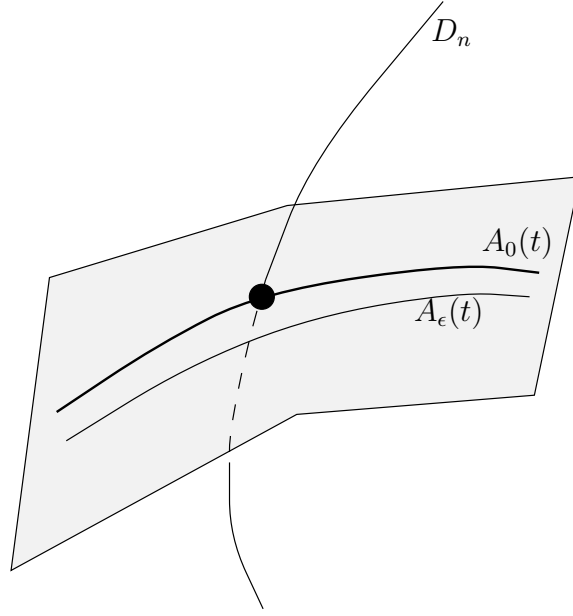


FIGURE 7. Avoided crossings

Under the hypothesis  $(\mathbf{H}_1)$ , we can reduce (31) to:

$$(32) \quad \frac{h}{i} \frac{dX}{dt} = \begin{pmatrix} \mu_1(t, \epsilon) + O(h) & w_0\epsilon + \omega_0 h + O(h^2 + \epsilon^2) \\ \bar{w}_0\epsilon + \bar{\omega}_0 h + O(h^2 + \epsilon^2) & \mu_2(t, \epsilon) + O(h) \end{pmatrix} X$$

where the non diagonal entries are **independent of  $t$** . This independance eliminates in the reduced form the troublesome case, where the non-diagonal entries tend to zero at  $t_0$ , which is possible in the original equation (31). It allows a clear cut distinction between effective, dynamical, crossing and avoided crossing cases, distinct from the mere crossing or avoided crossing of eigenvalues  $\lambda_1(t, \epsilon)$  and  $\lambda_2(t, \epsilon)$  of  $A_\epsilon(t)$ , which is precluded for  $\epsilon \neq 0$  by hypothesis  $(\mathbf{H}_1)$ . We are then able to apply theorem 4 in order to get a Landau-Zener-Friedrichs-Hagedorn formula. In this reduced equation  $w_0$  is related to the size of the minimal gap  $\text{gap}(\epsilon) = \inf |\lambda_1(t, \epsilon) - \lambda_2(t, \epsilon)|$  by  $\text{gap}(\epsilon) \sim 2|w_0\epsilon|$  and  $\omega_0$  to the infinitesimal rotation of a smooth basis  $(v_1(t), v_2(t))$  of eigenvectors of  $A_0(t)$  associated to  $\lambda_1(t)$  and  $\lambda_2(t)$  where  $\lambda_j(t_0) = \lambda_0$ ,  $j = 1, 2$ . More precisely:

$$w_0 = \langle G_0 v_2(t_0) | v_1(t_0) \rangle, \quad \omega_0 = i \langle v_2'(t_0) | v_1(t_0) \rangle.$$

**6.1. Reduction I: reduction to a 2-levels system.** We want to show that under hypothesis  $(\mathbf{H}_1)$ , we can reduce the  $N$ -levels system to a 2-levels system and then we will make a further reduction with  $t$ -independent non-diagonal term which allows to apply the theorem 4.

We have the following general result:

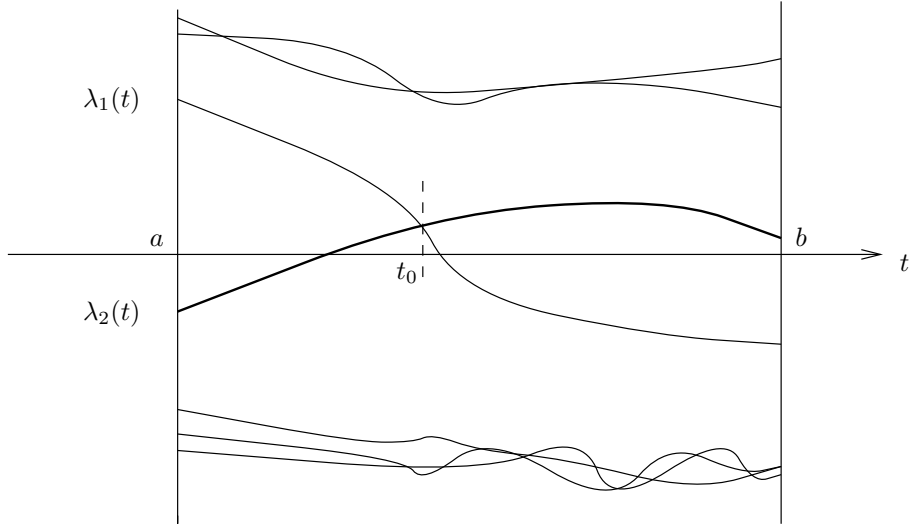


FIGURE 8. Phases portrait

**Theorem 5.** *Let us consider the following adiabatic system:*

$$(33) \quad \frac{\hbar}{i} \frac{dX}{dt} = A(t)X, \quad a \leq t \leq b$$

and assume that on the interval  $[a, b]$  the space  $\mathbb{C}^N$  do admit a smooth splitting

$$\mathbb{C}^N = E(t) \oplus F(t)$$

which is stable by  $A(t)$  and such that spectra of  $A(t)$  restricted to  $E(t)$  and  $F(t)$  are disjoint. Let us give a smooth unitary  $P_0(t)$  such that

$$(34) \quad P_0^{-1} A(t) P_0 = \begin{pmatrix} K_0(t) & 0 \\ 0 & L_0(t) \end{pmatrix}.$$

Then there exist formal series

$$P(t) = P_0(t) + \hbar P_1(t) + \dots$$

with  $P(t)$  unitary in  $\mathbb{C}^N$  and formal series with values into the Hermitian operators on  $E(t)$  (resp.  $F(t)$ )

$$K(t) = K_0(t) + \hbar K_1(t) + \dots, \quad L(t) = L_0(t) + \hbar L_1(t) + \dots$$

such that, if we define

$$X(t) = P(t)Y(t),$$

the equation (33) rewrites

$$(35) \quad \frac{\hbar}{i} \frac{dY}{dt} = \begin{pmatrix} K(t) & 0 \\ 0 & L(t) \end{pmatrix} Y(t) + O(\hbar^\infty) Y(t), \quad t \in [a; b].$$

We will, of course, apply theorem 5 to the case where  $A(t)$  depends on a parameter  $\epsilon$  such that hypothesis are fulfilled uniformly in  $\epsilon$ .

*Proof.*—

The proof is by induction: at the first step, we just take  $P_0(t)$  which reduces  $A(t)$  to two blocks. The resulting equation for  $Y(t)$  is

$$(36) \quad \frac{h}{i} \frac{dY}{dt} = \begin{pmatrix} K_0(t) & 0 \\ 0 & L_0(t) \end{pmatrix} Y(t) - \frac{h}{i} P_0^{-1}(t) P_0'(t) Y(t),$$

with a  $h$  remainder to eliminate. At step  $n$ ,  $P(t)$  is corrected by a factor  $e^{h^n S}$ . Diagonal order  $h^n$  terms correct  $K(t)$  and  $L(t)$ . Cancelling the non diagonal order  $h^n$  terms leads to solve the following homological equation

$$K_0 S_{EF} - S_{EF} L_0 = R$$

where  $R$  is given (the  $EF$  non diagonal part of the order  $h^n$  remainder of step  $n-1$ ). The hypothesis that the two spectra are disjoint allows to solve it. That result is well known, but it is difficult to find a precise reference in the literature, see however [17] p. 315 and ff.

□

It is possible to add the following refinement:

**Theorem 6.** *Let  $t_0 \in ]a, b[$  be such that, if we put  $E_0 = E(t_0)$ ,  $F_0 = F(t_0)$ , the restriction of  $A(t_0)$  to  $E_0$  is  $\lambda_0 \text{Id}$ . Let  $\Omega(t) = P_0^{-1}(t) P_0'(t)$  and  $\Pi$  the projection on  $E_0$  whose kernel is  $F_0$ . We have then*

$$K(t_0) = \lambda_0 \text{Id} + ih \Pi \Omega(t_0) \Pi + O(h^2) .$$

*If  $P_0$  is unitary and  $v_j(t) = P_0(t)(e_j)$ , the matrix of  $\Pi \Omega(t_0) \Pi$  is given by  $\omega_{i,j} = \langle v_i'(t_0) | v_j(t_0) \rangle$ . In particular, the  $v_j$ 's are defined up to some phase shift, their modules  $\omega_{i,j}$  are independent of the choice of  $P_0$  for  $i \neq j$ .*

It comes from an explicit computation: if we put  $X = (P_0 + hP_1 + O(h^2))Z$  and  $\Delta(t) = P_0(t)^{-1} A(t) P_0(t)$ , we get for  $Z$  the equation:

$$\frac{h}{i} \frac{dZ}{dt} = (\Delta(t) + ih\Omega(t) + h[\Delta(t), P_1(t)] + O(h^2))Z .$$

We deduce the result, using our hypothesis, because for all  $B$ , we have:

$$\Pi[\Delta(t_0), B]\Pi = 0 .$$

Using the theorem 5, we are reduced to study near an avoided eigenvalue crossing the following 2-levels system:

$$(37) \quad \frac{h}{i} \frac{dX}{dt} = \begin{pmatrix} \lambda_1(t) + k_{1,1}(t, h, \epsilon) & k_{1,2}(t, h, \epsilon) \\ k_{1,2}(t, h, \epsilon) & \lambda_2(t) + k_{2,2}(t, h, \epsilon) \end{pmatrix} X$$

where  $k_{i,j}(t, h, \epsilon)$ 's are formal series in  $(h, \epsilon)$ :

$$k_{i,j}(t) = \sum_{l+m \geq 1} k_{i,j;l,m}(t) h^l \epsilon^m .$$

We have moreover:

**Proposition 2.** *The hypothesis  $(\mathbf{H}_1)$  implies that  $k_{1,2;0,1}(t)$  does not vanish near  $t_0$ . Moreover  $|k_{1,2;1,0}(t_0)| = | \langle v'_1(t_0) | v_2(t_0) \rangle |$  is the infinitesimal rotation of the frame  $(v_1(t), v_2(t))$  at  $t = t_0$ .*

**6.2. Reduction II: reduction of the 2-levels system.** We want now to reduce the 2-levels system to a new 2-levels system with  $t$ -independent non diagonal entries.

Assuming hypothesis  $(\mathbf{H}_1)$ , we can assume that  $\Delta(t)$  is a diagonal matrix  $\Delta(t) = \text{diag}(\lambda_1(t), \lambda_2(t))$ . It is enough to look at the matrix

$$\frac{1}{t - t_0} (\Delta(t) - \lambda_0 \text{Id})$$

which is smoothly dependent on  $t$  and whose eigenvalues remain distinct. It shows that eigenvalues  $\lambda_j(t)$ ,  $j = 1, 2$ , and eigenvectors of  $A_0(t)$  are smooth.

Let

$$(38) \quad A_\epsilon(t) = \begin{pmatrix} a(t, \epsilon) & b(t, \epsilon) \\ \bar{b}(t, \epsilon) & d(t, \epsilon) \end{pmatrix}$$

be a  $2 \times 2$  Hermitian matrix which depends smoothly on  $(t, \epsilon)$  in some neighbourhood of  $(0, 0) \in \mathbb{R}^2$ . We assume the following hypothesis which follows from  $(\mathbf{H}_1)$ :

•

$$(39) \quad A_0(t) = \text{Diag}(\lambda_1(t), \lambda_2(t))$$

with  $\lambda_1(0) = \lambda_2(0)$  and  $\lambda'_1(0) > \lambda'_2(0)$ .

•

$$(40) \quad \frac{d}{d\epsilon} (A_\epsilon(t))|_{t=\epsilon=0} = \begin{pmatrix} A & B \\ \bar{B} & C \end{pmatrix}$$

and  $B \neq 0$ .

Then we have the following:

**Lemma 3.** *There exists a smooth function  $\gamma(\epsilon)$  with  $\gamma(0) = 0$ ,  $\gamma'(0) > 0$  (in fact  $\gamma'(0) = |B|$ ) such that*

$$(41) \quad |2\gamma(\epsilon)| = \inf_t |\lambda_2(t, \epsilon) - \lambda_1(t, \epsilon)| ,$$

where the  $\lambda_j(t, \epsilon)$  denotes the eigenvalues of  $A_\epsilon(t)$ .



There exists a unique smooth map  $(t, \epsilon) \rightarrow U_\epsilon(t)$  from a neighbourhood of  $(0, 0)$  into the unitary matrices

$$(42) \quad U_\epsilon(t) = \begin{pmatrix} c & -\bar{s} \\ s & c \end{pmatrix}$$

which satisfy  $c > 0$ ,  $U_0(0) = \text{Id}$  and

$$(43) \quad U_\epsilon^*(t) A_\epsilon(t) U_\epsilon(t) = \begin{pmatrix} \mu_1(t, \epsilon) & \gamma(\epsilon) \\ \gamma(\epsilon) & \mu_2(t, \epsilon) \end{pmatrix} =: \tilde{A}_\epsilon(t)$$

and  $\mu_j(t, 0) = \lambda_j(t)$ . The important fact is that  $\gamma(\epsilon)$  is independent of  $t$ .

*Proof.*—

The strategy of the proof is to build first  $\gamma(\epsilon)$  and  $\mu_j(t, \epsilon)$ , then to prove that both are smooth, that  $U_\epsilon(t)$  is uniquely defined outside  $(0, 0)$ , and finally to show that  $c$  and  $s$  are smooth.

If we define  $\varphi_\epsilon(t) = (\lambda_1(t, \epsilon) - \lambda_2(t, \epsilon))^2$ , the functions  $\varphi_\epsilon$  depend smoothly on  $\epsilon$ , and  $\varphi_0$  has a non degenerate minimum at  $t = 0$ . The same is true for  $\epsilon$  small and we denote  $t(\epsilon)$  the point where this minimum is obtained. We set  $4\gamma(\epsilon)^2 = \varphi_\epsilon(t(\epsilon)) := \psi(\epsilon)$ . Now it is clear that  $\psi(0) = 0$ ,  $\psi'(0) = 0$  and  $\psi''(0) > 0$ ; so we can choose a smooth square root  $2\gamma(\epsilon)$ . The same kind of argument shows that  $\mu_j(t, \epsilon)$  are smooth: we ask that  $A_\epsilon$  and  $\tilde{A}_\epsilon$  have the same eigenvalues. It gives  $\mu_1 + \mu_2 = a + c$  and  $(\mu_1 - \mu_2)^2 = (\lambda_1 - \lambda_2)^2 - 4|\gamma|^2$ . This last function of  $t$  is positive and admits 0 as a non degenerate minimal value. It implies that it is the square of a smooth function and so that  $\mu_j$  can be chosen smooth and  $\mu_j(t, 0) = \lambda_j(t)$ .

The existence and uniqueness of  $U_\epsilon(t)$  come from the fact that both matrices  $A_\epsilon(t)$  and  $\tilde{A}_\epsilon(t)$  are conjugated by a unique  $U$  with  $c > 0$  (they have the same eigenvalues).

Now  $(c, s)$  satisfy

$$(d - \mu_1)s = (\gamma - \bar{b})c.$$

This equation admits a solution because we know already that both matrices are conjugated, hence  $\gamma - \bar{b}$  vanishes where  $d - \mu_1$  does. It is now enough to check that the differential of  $d - \mu_1$  is not zero at the point  $t_0$ . We have

$$\frac{\partial}{\partial t}(d - \mu_1) = \frac{\partial}{\partial t}(\lambda_2 - \lambda_1),$$

which is non zero by hypothesis.

□

From that lemma, we deduce that:

**Theorem 7.** *The reduced adiabatic system can be written in a smooth ONB as:*

$$(44) \quad \frac{h}{i} \frac{dX}{dt} = \left( \begin{pmatrix} M_1(t, \epsilon, h) & \Gamma(\epsilon, h) \\ \bar{\Gamma}(\epsilon, h) & M_2(t, \epsilon, h) \end{pmatrix} + O(h^\infty) \right) X$$

where  $M_j$  are symbols in  $h$  of the form

$$M_j(t, \epsilon, h) = \mu_j(t, \epsilon) + \sum_{k=1}^{\infty} \mu_{j,k}(t, \epsilon) h^k$$

and  $\Gamma(\epsilon, h)$  is a symbol of the form

$$\Gamma(\epsilon, h) = \gamma(\epsilon) + \sum_{k=1}^{\infty} \gamma_k(\epsilon) h^k .$$

The important fact is that  $\Gamma(\epsilon, h)$  is independent of  $t$ .

*Proof.*—

The proof is by induction on the powers of  $h$ . We start with an equation

$$(45) \quad \frac{h}{i} \frac{dX}{dt} = \left( \begin{pmatrix} M_1(t, \epsilon, h) & \gamma(\epsilon) + h\alpha_1(\epsilon, t) + O(h^2) \\ \bar{\gamma}(\epsilon) + h\bar{\alpha}_1(\epsilon, t) + O(h^2) & M_2(t, \epsilon, h) \end{pmatrix} \right) X$$

and we put at the first step

$$X = (\text{Id} + ihP)Y$$

where

$$(46) \quad P = \begin{pmatrix} 0 & \pi(\epsilon, t) \\ \bar{\pi}(\epsilon, t) & 0 \end{pmatrix}$$

By asking to make  $\alpha_1(t, \epsilon)$  independent of  $t$ , we get then an homological equation

$$i(\mu_1(t, \epsilon) - \mu_2(t, \epsilon))\pi(t, \epsilon) + \alpha_1(t, \epsilon) = \gamma_1(\epsilon) .$$

We choose  $\gamma_1(\epsilon)$  as the value of  $\alpha_1(t, \epsilon)$  at the point where  $\mu_1 = \mu_2$  and we get a smooth  $\pi$ .

□

**6.3. The Landau-Zener-Friedrichs-Hagedorn formula.** Using theorem 7, we have the following extension of Landau-Zener and Friedrichs-Hagedorn formulae:

**Theorem 8.** *Assuming hypothesis  $(\mathbf{H}_1)$ , we have the following asymptotic expansion for the reduced  $T = (t_{i,j})$  matrix:*

$$|t_{1,2}| = |t_{3,4}| + O(h^\infty) = e^{\pi\Phi(\epsilon, h)/h} + O(h^\infty) .$$

where  $\Phi$  satisfies:

$$\Phi(\epsilon, h) = -\frac{|\epsilon w_0 + h\omega_0|^2}{|\lambda'_1(t_0) - \lambda'_2(t_0)|} + O((|h| + |\epsilon|)^3) .$$

*Proof.*—

The proof is just an application of theorem 1 to the equation

$$(P_2 P_1 - |\Gamma|^2)u = 0$$

where  $P_j = \frac{h}{i} \frac{d}{dt} - M_j(t, \epsilon, h)$  and  $u$  is the first component of our unknown function. In this reduction from matrix to scalar equation for  $u$ , we use fully the fact that  $\Gamma$  is  $t$ -independent.

□

## 7. EXTENSIONS AND REMARKS

**7.1. Phases.** The Landau-Zener formula does not provide enough information in order to compute the semi-classical limit when there are several avoided crossings. In that case, one should look at phases. In the case of a scalar equation, a similar problem is solved in [8]. The case of systems will be described in [5]. That way, we can compute the semi-classical spectrum of a system of weakly coupled Schrödinger operators (Born-Oppenheimer approximation in dimension 1). In the adiabatic case, we are also able to compute the scattering matrix and to describe the *Stückelberg's* oscillations as in ([19] p. 241).

**7.2. Time dependent case.** Let us just give the intuition behind. The classical limit of the Schrödinger system

$$(47) \quad \frac{h}{i} \frac{d}{dt} \begin{pmatrix} u \\ v \end{pmatrix} = A \begin{pmatrix} u \\ v \end{pmatrix}$$

can be described as follows: on the energy shell  $E$ , we have two independent Hamiltonian systems associated respectively to  $p_1$  and to  $p_2$ . The energy shell  $E$  is the disjoint union of the curves  $X_1 = \{p_1 = E\}$  and  $X_2 = \{p_2 = E\}$ . If the trajectory on  $X_1$  or  $X_2$  passes through a crossing point  $z_0$ , we get a probabilistic dynamics with transition probabilities from  $X_1$  to  $X_1$  or  $X_2$  given by the Landau-Zener formula. The classical limit is in fact a stochastic process!

In order to make some more precise statement, we need to use the small parameter version of the Guillemin-Melrose-Uhlmann theory of singular FIO associated to pairs of Lagrangian manifolds which have a clean intersection (see [20], [10], [27]).

## REFERENCES

- [1] J.E. Avron, A. Elgart, The Adiabatic Theorem in Quantum Mechanics. *Preprint mp-arc* 98-370 (1998).
- [2] M. Born, V. Fock, Beweis des Adiabatenatzes. *Z. Phys.*, 51:165-169 (1928).

- [3] P.J. Braam and J.J. Duistermaat, Normal forms of real symmetric systems with multiplicity. *Indag. Math.*, 4:407-421 (1993).
- [4] M. Carré, A. Zgainsky, M. Gaillard, M. Nouh, M. Lombardi, Détermination des populations relatives des sous-niveaux magnétiques du niveau  $4\ ^1D$  de  $HeI$  excité par impact d'ions lourds, *Journal de Physique*, 42:235-246 (1981).
- [5] Y. Colin de Verdière, Limite adiabatique en présence de croisements évités et phases géométriques. *En préparation*, (1998).
- [6] Y. Colin de Verdière and B. Parisse, Equilibre instable en régime semi-classique : I—Concentration microlocale. *Commun. PDE*, 19:1535-1563 (1994).
- [7] Y. Colin de Verdière and B. Parisse, Equilibre instable en régime semi-classique : II—Conditions de Bohr-Sommerfeld. *Ann. Inst. Henri Poincaré (Physique théorique)*, 61:347-367 (1994).
- [8] Y. Colin de Verdière and B. Parisse, Singular Bohr-Sommerfeld rules, *Prépublication de l'Institut Fourier no 432 (1998)*, à paraître dans *Commun. Math. Phys.*.
- [9] Y. Colin de Verdière and J. Vey, Le lemme de Morse isochore *Topology*, 18:283-293 (1979).
- [10] V. Guillemin, G. Uhlmann, Oscillatory integrals with singular symbols, *Duke Math. J.*, 48:251-267 (1981).
- [11] G. Hagedorn, Adiabatic Expansions near Eigenvalue Crossings. *Annals of Physics*, 196:278-295 (1989).
- [12] G. A. Hagedorn, Proof of the Landau-Zener formula in an adiabatic limit with small eigenvalue gap, *Commun. Math. Phys.*, 136:433-449 (1991).
- [13] G. A. Hagedorn, Molecular Propagation through Electron Energy Level crossings, *Memoirs of the AMS*, 536 (1994).
- [14] G. A. Hagedorn and A. Joye, Landau-Zener Transitions through small electronic eigenvalue gaps in the Born-oppenheimer approximation *Ann. IHP (physique théorique)*, 68:85-134 (1998).
- [15] A. Joye, Proof of the Landau-Zener formula, *Asymptotic Analysis*, 9:209-258 (1994).
- [16] A. Joye, Exponential asymptotics in a singular limit for  $n$ -level scattering systems, *SIAM J. Math. Anal.*, 28:669-703 (1997).
- [17] S.G. Krein, Linear Differential Equations in Banach Space. *Translations of Math. Monographs (AMS)* (1971).
- [18] L. Landau, *Collected papers of L. Landau*, Pergamon Press (1965).
- [19] P. Martin and G. Nenciu, Semi-classical inelastic  $S$ -matrix for one dimensional  $N$ -states systems, *Reviews in Mathematical Physics*, 7:193-242 (1995).
- [20] R. Melrose and G. Uhlmann, Lagrangian intersection and the Cauchy problem, *Comm. Pure Appl. Math.*, 32:483-519 (1979).
- [21] A. Messiah, *Mécanique quantique*, Dunod (1969).
- [22] J. Pollet, Analyse semi-classique d'un système d'équations de Schrödinger couplées : formule de Landau-Zener. *Thèse de l'université de Grenoble 1* (octobre 1997).
- [23] D. Robert, *Autour de l'approximation semi-classique*, Birkhäuser (1987).
- [24] H. Rosenthal, Nonadiabatic Effects in Slow Atomic Collisions. I.  $He^+ + He$ , *Phys. Rev.*, A4:1030-1042 (1971).
- [25] M. Rouleux, Feshbach resonances in the semi-classical limit, *Preprint CPT* (1997).
- [26] E.C.G. Stueckelberg, *Helv. Phys. Acta*, 5:369 (1932).
- [27] M. Taylor, Pseudo-differential operators, *Princeton* (1981).
- [28] W. Wasow, Asymptotic Expansions for Ordinary Differential Equations. *Wiley, New-York* (1985).
- [29] C. Zener, Non-adiabatic crossing of energy levels, *Proc. Roy. Soc. Lond.*, 137:696-702 (1932).